

Kinetic study of butenedial with the main atmospheric oxidants

P. Martín, I. Colmenar, B. Cabañas, M. S. Salgado, E. Martínez and A. Tapia.

*Departamento de Química Física, Facultad de Ciencias Químicas, Universidad de Castilla La Mancha.
Avda Camilo José Cela 10, 13071 Ciudad Real (Spain).*

Butenedial, (OHCCH=CHCHO), has been identified as a primary product from the reaction of furan with the main atmospheric oxidants, chlorine(1), OH (2) and NO₃ (3) Butenedial has also been detected after the OH photo-oxidation of reactive aromatic compounds such as toluene and o-xylene(4).

The degradation reactions of trans-2-butenedial with OH, NO₃ radicals and Cl atoms were investigated using a relative rate method. The experiments were carried out at $\sim 298 \pm 1$ K and atmospheric pressure of N₂ or synthetic air as bath gas. Two different sampling/detection methods have been used for the study with Cl and OH: (1) Solid-Phase Microextraction and gas chromatography with flame ionization detection (SPME/GC-FID) and (2) "in situ" with long path Fourier Transform Infrared Spectroscopy (FTIR). In the case of NO₃ study Tenax solid adsorbent was used as sampling method and gas chromatography with Mass Spectrometry (GC-MS) as detection system. The measured rate coefficients for E-2-butenedial (cm³ molecule⁻¹ s⁻¹) are: $(1.20 \pm 0.28) \times 10^{-10}$ for Cl atoms, $(3.44 \pm 0.30) \times 10^{-11}$ for OH radical and $(1.77 \pm 0.72) \times 10^{-15}$ for NO₃ radical. For the reaction of Cl and NO₃ these are the first data of rate coefficients and in the case of OH the literature value was confirmed(5). The results confirm that the chemical characteristics of the organic substances have a limited influence on the reactivity with Cl, a larger effect in the OH-case but are decisive for the NO₃ reactions. Calculated atmospheric lifetime with each atmospheric oxidant is 8 days and 8 hours for Cl and OH respectively. In the case of Cl atoms a lifetime of 19 hours is estimated in the early morning hours in urban coastal air.

1. Villanueva F, Barnes I, Monedero E, Salgado S, Gómez V and Martín P, *Atmospheric Environment*, **2007**, 41, 8796.
2. Gómez-Álvarez E, Borrás E, Viidanoja J and Hjorth J, *Atmospheric Environment*, **2009**, 43, 1603.
3. Berndt T, Böge O and Rolle W, *Environmental Science Technology*, **1997**, 31, 1157.
4. Arey J, Obermeyer G, Aschamann S. M, Chattopadhyay S, Cusick R D. and Atkinson R *Environmental Science Technology*, **2009**, 43, 683.
5. Bierbach A, Barnes I, Becker K.H and Wiesen E, *Environmental Science and Technology*, **1994**, 28 (4), 715.